$[X^{\hat{1}}MT_{F}X-Tips 130208a-pdf]$

Disaccharides—Sugars

Shinsaku Fujita Shonan Institute of Chemoinformatics and Mathematical Chemistry

February 8, 2013

Question:

How can I draw sugars by using XÎMT_EX?

Answer:

The commands \furanose and \pyranose are supported by \hat{X}\text{MTEX} to draw monosaccharides. They are combined by using (yl) functions. The following code is effective in the plain mode of \hat{X}\text{MTEX}, the PostScript mode, and the PDF mode.

```
%130208a-pdfTest.tex
\documentclass{article}
%\usepackage{xymtex}%plain mode
%\usepackage{xymtexps}% PostScript mode ... followed by dvips(k)
\usepackage{xymtexpdf}% PDF mode ... followed by dvipdfmx
\begin{document}
\utrigonal{0==0;2==%}
\furanose{4==(y1);1Sa==CH$_{2}$0H;2Sb==\lmoiety{H0};%
2Sa==H;3Sb==H;3Sa==0H;4Sb==HOC\rlap{H$_{2}$};%
3==\pyranose{1==(y1);2Sa==0H;3Sb==OH;4Sa==HO;5Sb==CH$_{2}$OH}}
```

\end{document}

The present XyMTeX-tip deals with the PDF mode. The code named "130208a-pdfTest.tex" is executed by \LaTeX as follows:

c:\> latex 130208a-pdfTest

The resulting .dvi file is converted into the corresponding .pdf file:

c:\> dvipdfmx 130208a-pdfTest

Thereby, we obtain a .pdf file ("130208a-pdfTest.pdf"), which contains the following structural formula of a disaccharide.

The .pdf file is browsed by the Adobe Reader.

Further Techniques

The same formula can be drawn by using lower-level commands \fivesugarh and \sixsugarh, which are capable of specifying the position of an oxygen atom in each sugar skeleton.

```
\label{lem:constraint} $$ \displaystyle 10=0;2==\% \\ fivesugarh{5==0}_{4==(y1);1Sa==CH$_{2}$0H;2Sb==\\lmoiety{H0};\% \\ 2Sa==H;3Sb==H;3Sa==0H;4Sb==H0C\\rlap{H$_{2}$};\% \\ 3==\\sixsugarh{6==0}_{1==(y1);2Sa==0H;3Sb==0H;4Sa==H0;5Sb==CH$_{2}$0H} \}
```

$$\begin{array}{c} CH_2OH \\ O \\ OH \\ OH \\ OH \\ OH \\ H \end{array}$$

Inner wedged bonds can be drawn by using the \WedgeAsSubst command. The following code uses the \draw command of the pgf package.

```
\utrigonal{0==0;2==%
\fivesugarh{5==0;1s==\WedgeAsSubst(0,0)(-3,-5){120};%

4s==\WedgeAsSubst(0,0)(3,-5){120};%

3s==\tikznodimension{\draw[line width=2.9pt]%
(-17\unitlength,0) -- (307\unitlength,0);}%
\}{4==(y1);1Sa==CH$_{2}$0H;2Sb==\lmoiety{H0};2Sa==H;%
3Sb==H;3Sa==0H;4Sb==HOC\rlap{H$_{2}$}\[abc];%
3==\sixsugarh{6==0;1s==\WedgeAsSubst(0,0)(-3,-5){120};%
4s==\WedgeAsSubst(0,0)(3,-5){120};%
3s==\tikznodimension{\draw[line width=2.9pt]%
(-17\unitlength,0) -- (307\unitlength,0);}%
\}{1==(y1);2Sa==0H;3Sb==OH;4Sa==H0;5Sb==CH$_{2}$OH}[abc]}
```

$$\begin{array}{c} CH_2OH \\ O \\ HO \\ OH \\ OH \\ OH \\ H \\ \end{array}$$

In place of the \draw command of the pgf package, a more general command \PutBondLine can be used in the PDF mode as well as in the PostScript mode. Thus, the following code is processed by the PDF mode of \X^2MT_FX .

```
\utrigonal{0==0;2==%
\fivesugarh{5==0;1s==\WedgeAsSubst(0,0)(-3,-5){120};%

4s==\WedgeAsSubst(0,0)(3,-5){120};%

3s==\PutBondLine(-15,0)(305,0){3.2pt}%
\}{4==(y1);1Sa==CH$_{2}$0H;2Sb==\lmoiety{H0};2Sa==H;%

3Sb==H;3Sa==0H;4Sb==HOC\rlap{H$_{2}$}\[abc];%

3==\sixsugarh{6==0;1s==\WedgeAsSubst(0,0)(-3,-5){120};%

4s==\WedgeAsSubst(0,0)(3,-5){120};%

3s==\PutBondLine(-15,0)(305,0){3.2pt}%
\}{1==(y1);2Sa==0H;3Sb==OH;4Sa==H0;5Sb==CH$_{2}$OH}[abc]}
```

Thereby, we obtain the same formula of the sugar as depicted above:

$$\begin{array}{c} CH_2OH \\ O \\ HO \\ OH \\ OH \\ OH \\ H \\ HO \\ CH_2OH \\ \end{array}$$